Quantized vortex reconnection: Fixed points and initial conditions

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Quantized vortices are phase singularities in complex fields. In superfluids, they appear as mobile interacting defects that may cross and reconnect by exchanging tails. Reconnection is a topology-changing event that allows vortex tangles to decay; it is a defining signature of quantum turbulence. We report a family of fixed points (i.e., stationary solutions), including planar forms, that capture reconnection in the Gross-Pitaevskii model in contrast to previous suggestions of pyramidal structures. These are obtained using a well known, systematic method for generating low-energy relaxed initial conditions for Gross-Pitaevskii simulations.

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Quantized vortex reconnection is a topology-changing mechanism by which two quantized vortices in a quantum fluid (e.g., superfluid ^{4}He) approach and exchange tails.[1] Reconnection is important as a decay mechanism in quantum turbulence,[2–4] and has recently been directly observed experimentally.[5] It was found that reconnection events were involved in strongly non-Gaussian velocity statistics, clearly distinguishing quantum from classical turbulence.[5]

A quantized vortex exists as a line phase defect on the locus of zeros of both the real and imaginary parts of a complex field Ψ. In the context of superfluids, Ψ is the order parameter, often taken to obey the Gross-Pitaevskii (GP) equation. The GP equation, which naturally exhibits quantized vortex solutions and reconnection, has received much theoretical and numerical examination as a useful model of superfluids and Bose-Einstein condensates. Quantized vortices are also of widespread interest in other processes that have topological defects, such as Ginzberg-Landau theory, superconductivity,[6] liquid crystals, and cosmic strings. Magnetic reconnection is a closely related and similarly active field of study in plasmas and astrophysical magnetohydrodynamics.[7]

Many interesting and significant numerical studies have investigated quantized vortex evolution and reconnection,[8–15] but have not often explored in detail the role of the initial data. Given the Hamiltonian structure of GP evolution, and that the three dimensional (3D) equation conserves total energy, momentum, and mass, it is not surprising that initial data are central to the dynamics. Here we present evidence of the important role of initial data on vortex evolution.

This paper presents a method for generating well-specified initial conditions and, as a cautionary tale, the unintended results of failing to do so. A method is recalled,[16] which we exploit to find previously unidentified fixed points, that is stationary solutions of the underlying Hamiltonian dynamics, relevant to vortex reconnection. Recent analytical work on the topology of complex fields with connections to the results of previous work on linear models of reconnection[17] and our fixed points is also discussed.

Theoretical studies of complex fields[18] provide generic descriptions and a classification of phase singularities and topology-changing events of which vortex reconnection is but one example. Indeed, distinct categories have been established which have direct analogs in the context of superfluids with a single straight vortex, the reconnection of vortices, and ring propagation, generation, and decay. Specifically, Berry and Dennis[18] have precisely defined the conditions required in a complex field for a topology-changing event to occur. They provide a general Taylor expansion of a complex field Ψ near a topology-changing event, namely,

$$\Psi(x,y,z;t) = t + i(az) + \tfrac{1}{2}\mathbf{r}\cdot\mathbf{A}\cdot\mathbf{r} + O(r^4) \qquad (1)$$

with a bifurcation on a real time parameter which unfolds the singularity. Here a is a scalar, $\mathbf{r} = (x,y,z)$, and $\mathbf{A}$ is a complex, symmetric 3×3 matrix. They show that if $\det\{\mathrm{Re}\ \mathbf{A}\} > 0$ the process is elliptical and analogous to a vortex ring which shrinks and vanishes. If $\det\{\mathrm{Re}\ \mathbf{A}\} < 0$ the process is hyperbolic and analogous to a pair of vortices that reconnect. These are the only two stable topology-changing events in complex fields,[18] and their analogous physical processes in superfluid ^{4}He have both been observed in experiment.[5] This supports the idea that topology-changing events are deeply involved with quantum turbulence decay.

It is worth noting that (1) encapsulates our analytic work presented below and the linear aspects of the well-known study of Nazarenko and West[17] on vortex reconnection. The analysis by Berry and Dennis was executed in the context of optical vortices but is generally applicable to all systems with an evolving complex field; it can be helpful in understanding quantized vortices. Here we focus on the hyperbolic case associated with vortex reconnection.

The Gross-Pitaevskii Equation (GPE) may be written

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(\frac{-\hbar^2}{2m}\nabla^2 - \mu + \gamma|\Psi|^2\right)\Psi, \qquad (2)$$

and expressed in dimensionless form using natural time and space units, (t_0,ξ_0), yielding $\partial/\partial\bar{t} = (\hbar/\mu)\partial/\partial t$, $\bar{\nabla} = \hbar/\sqrt{2m\mu}\,\nabla$, and $\bar{\Psi} = \Psi/\sqrt{m\mu}$. For ^{4}He, accepting a healing length $\xi_0 \approx 0.9$ Å gives $t_0 \approx 0.5$ ps.

To prepare minimal-energy initial conditions and to re-examine the straight vortex solution, we employ the diffusive GP equation (DGPE), with a real diffusivity, written in dimensionless form as

$$\frac{\partial \Psi}{\partial t} = (\nabla^2 + 1 - |\Psi|^2)\Psi. \tag{3}$$

Notice that a stationary solution of the DGPE is simultaneously a *fixed point* for the GPE. This fact can be exploited to find fixed points of the GPE numerically, and to generate relaxed, minimal-energy initial conditions for dynamical GPE simulations with a specified initial phase profile. The procedure is analogous to the imaginary-time propagation method,[16] used in Bose-Einstein condensate theory and simulations to study the ground states.

To perform any vortex calculation using the GPE, a vortical initial condition must be specified. An infinite straight vortex is an axisymmetric stationary solution of the GPE that is expressible in cylindrical spatial coordinates as

$$\Psi(r,\phi,z) = f(r)e^{i\phi}, \tag{4}$$

where the density profile satisfies $f(r) \to 0$ when $r \to 0$, and $f(r) \to 1$ when $r \to \infty$. Since there are no exact analytical forms for $f(r)$, it must be found numerically; but this is not practical when a wave function for multiple vortices is required as an initial condition. In previous work, it has been customary to use some convenient analytic but approximate density profile,[10–12,15] and to multiply such wave functions together, one for each vortex, to construct a $\Psi_0 \equiv \Psi(\mathbf{r},t=0)$.

We propose a systematic method for generating an initial condition of minimal energy by using the DGPE. First, one generates an approximate *phase profile* $\phi_0(\mathbf{r})$, defined throughout the computational domain, that qualitatively describes the desired initial vortex configuration. Then a corresponding initial wave function Ψ_0 with phase factor $e^{i\phi_0(\mathbf{r})}$ is constructed. This is evolved via the DGPE, (3), allowing the magnitude $|\Psi(\mathbf{r},t)|$ to diffuse, but actively maintaining the same, fixed phase profile, i.e., $\phi_0(t) = \tan^{-1}(\mathrm{Re}\{\Psi_0\}/\mathrm{Im}\{\Psi_0\})$. This process converges to a relaxed solution with minimal energy and provides reproducible low-energy initial data for a GP calculation. Note that the Lyapunov functional of the DGPE, which can only decrease or become stationary, is identical to the Hamiltonian for the GP model. For a single straight vortex along the z axis, $\Psi_0 = (x+iy)/\sqrt{x^2+y^2}$ is a sufficient input and converges to the minimal-energy relaxed core density profile. Multiple-vortex initial conditions can be generated by parameterizing the single-vortex phase factors for each desired vortex, multiplying these together, and diffusing as above. The technique will be elaborated in a future manuscript.

The consequences of using conventional approximate density profiles are dramatic. Figure 1 compares three of these analytical forms, namely, the Kerr,[15] Fetter,[19] and Berloff[13] approximants, showing how they differ, some substantially, from the relaxed numerical solution found by first evolving with the DGPE or, equivalently, by numerically solving the relevant radial ordinary differential equation for $f(r)$.[8] The Kerr and Fetter approximants launch strong radial waves when imposed as initial conditions for a single straight vortex and evolved in a GP computation. The emission arises as the inner core region evolves towards the relaxed density profile while the excess energy propagates outwards as waves: see Fig. 2. This is clearly a mistaken consequence of not specifying minimal-energy initial conditions. (Of course, an interesting

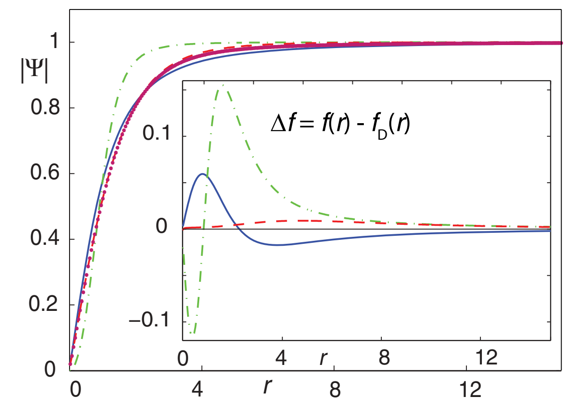

FIG. 1. (Color online) Comparison of approximate density profiles, $|\Psi| = f(r)$, as introduced by Kerr[15] $f_K^2 = r^4/(2+r^4)$ (green, dot-dashed), proposed by Fetter[19] $f_F^2 = r^2/(2+r^2)$ (blue, solid), and developed by Berloff[13] $f_B^2 = 11r^2(12+r^2)/(384+182r^2+11r^4)$ (red, dashed), with the diffused/exact profile $f_D(r)$ (pink, dotted). The inset displays the differences, $f_B(r)$ being closest to the exact stationary solution with lowest energy per unit mass. Relative to f_D the excess energies are about 6%, 2%, and 1%, respectively.

feature of the reconnection of vortices is the generation of acoustic waves, etc.; see, e.g., Secs. 4 and 5 of Ref. 12) Any of the three approximate profiles can be relaxed to a stable, minimal-energy solution, by first using the DGPE technique.

Using these same methods we can find fixed points of the GPE representing the specific moment of reconnection. The simplest of these we call Ψ_4, here shown schematically in Fig. 3(a). This vortex configuration is poised to reconnect into the 1st and 3rd (x,y) quadrants, as in Fig. 3(c), or into the 2nd and 4th. This bistability underlies the saddle nature of the time dynamics near the fixed point.

The local linear structure of this reconnection fixed point is, using an auxiliary length parameter η,

$$\Psi_4(x,y,z) \approx xy + i(\eta z). \tag{5}$$

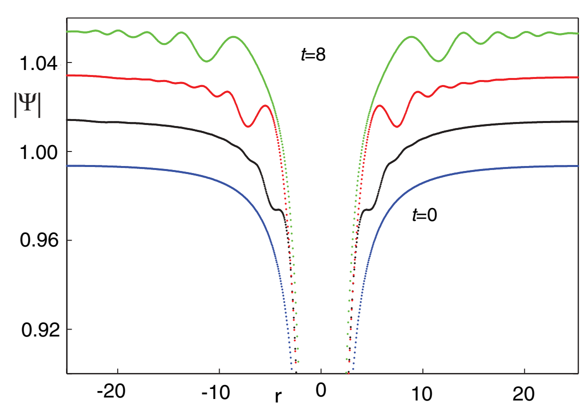

FIG. 2. (Color online) Time evolution of the Fetter approximant for a single straight stationary vortex according to the GPE integrated in a periodic domain: $f_F = |\Psi|$ is plotted at times $t = 0,2,4,8$ along a midplane section. To reveal the time evolution, successive profiles have been shifted. Evidently, the density profile f_F is not a minimal-energy condition and immediately launches erroneous acoustic waves.

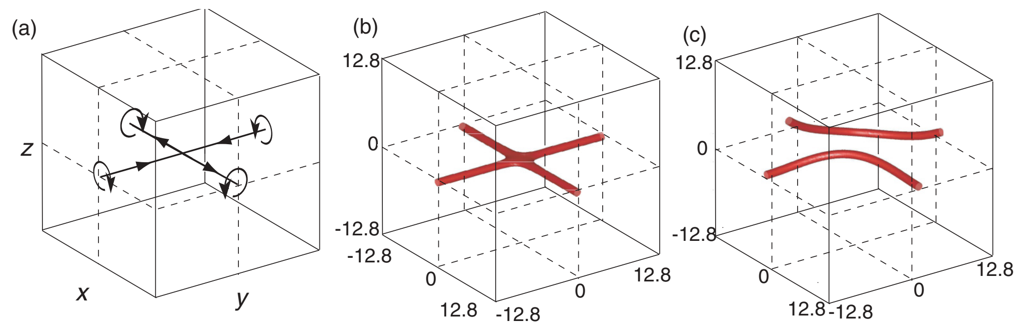

FIG. 3. (Color online) The Ψ_4 reconnection fixed point is shown schematically in (a). It consists of four half-infinite coplanar vortices meeting at right angles. Isosurfaces of the fixed point at $|\Psi_4| = 0.3$ are shown in (b), as obtained via the diffusive GP equation. The fixed point is, dynamically, an exponentially unstable saddle that, after a minimal white-noise perturbation in a time-dependent GP solver, develops with time in a box of size $L = 24.6$ as shown in part (c).

This determines the phase profile for the four half-infinite vortices shown in Fig. 3(a). We extend this lowest order Taylor series model (a fixed point of the linearized GPE) to a full nonlinear GPE solution by using the DGPE as above. The phase profile implied by (5) was held constant in a DGPE solver until the fully converged fixed-point solution in Fig. 3(b) emerged. This was done in an $L \times L \times L$ Cartesian box, using 4th order Runge-Kutta time integration and 2nd order centered finite differences for the Laplacian operator. The length parameter η was set to $L/2$ which served to produce circular vortex cores. With $\hat{n}$ a unit vector normal to a box wall, we set $(\nabla\Psi)\cdot\hat{n} = 0$ for each wall, to enforce no-flux boundary conditions. In relaxing the initial $\Psi(\mathbf{r})$ it proved necessary to enforce all symmetries: thus the functional form in (5) satisfies $\mathrm{Re}\{\Psi(x,y,z)\} = -\mathrm{Re}\{\Psi(-x,y,z)\} = \mathrm{Re}\{(-x,-y,z)\}$, etc. To protect the calculation from symmetry-breaking instabilities fed by roundoff, corresponding values were averaged and reassigned in the box at each time step.

The resulting Ψ_4 fixed point, shown in Fig. 3(b), constitutes a counterexample to a suggested[1] universal reconnection with a fixed 3D pyramidal form; see also Tebbs *et al.*[14] Note (5) is a specific example of a hyperbolic phase singularity in a complex field as discussed by Berry and Dennis.[18] Nazarenko and West[17] also discussed reconnection in hyperbolic configurations: their analysis includes (5) as a special case of a family of *linear* solutions, parametrized by the opening angle between the four half-vortices. Indeed, their perpendicular linearized configuration is *likewise* stationary.

To study the dynamics about our Ψ_4 fixed point, the final DGPE solution was perturbed by white noise of order 10^{-4} at each grid point in the GP solver, and evolved in time, yielding configurations as illustrated in Fig 3(c). The fixed point proves exponentially unstable with a unique, positive, real eigenvalue λ. The L_2 deviation from the fixed point, namely, $\delta_{L2}(t) = V^{-1}\int_V d^3r|\Psi(t) - \Psi_4|^2$, grows exponentially as $e^{\lambda t}$: see the log-linear inset in Fig. 4. The eigenvalue λ depends quite strongly on the box size L, measured in

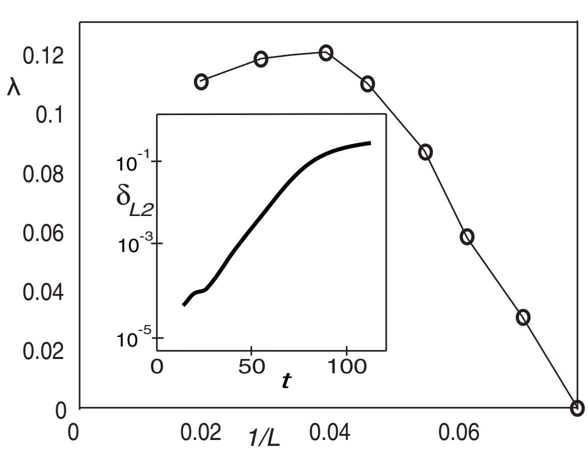

FIG. 4. The eigenvalue λ of the fixed point Ψ_4 varies with the size of the computational box L. The inset illustrates an exponential L_2 growth after a small perturbation of the fixed point Ψ_4 in a box of size $L = 24.6$.

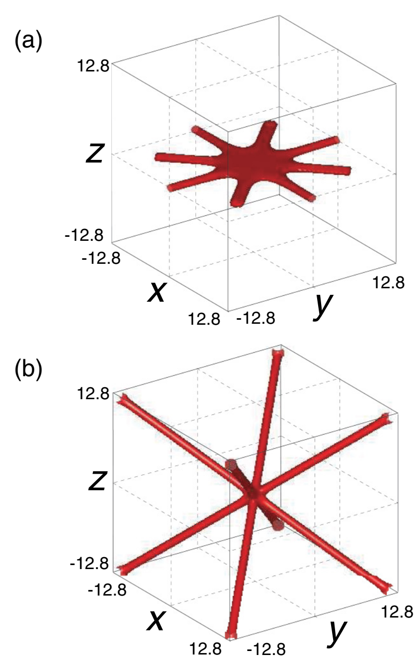

FIG. 5. (Color online) Two higher-order fixed points found numerically: (a) the planar eight half-vortex form (6) and (b) the three-dimensional body centered cubic form (7). The $|\Psi| = 0.3$ isosurfaces are shown.

terms of the healing length ξ_0, as seen in Fig. 4; indeed, quantitatively reliable dynamics requires computational box sizes $L > 25$.

Fixed points of the GPE involving straight half-vortices meeting at a point can also be regarded as satisfying a geometric "advection analysis." Each vortex core generates a solenoidal velocity field, with direction given by the vortex sign, either "inwards" or "outwards." For a fixed point, the mutual advection of each half-vortex on every other half-vortex must sum to zero. Contemplating these criteria, we have found several other fixed point geometries. Because these higher-order fixed points involve many vortices meeting at a point, they are improbable in real flows of a quantum fluid, unless symmetry constraints are imposed. However, the fixed points are of some interest for small physical systems, and, furthermore, they demonstrate the ability to find fixed points of higher order.

We have confirmed numerically that eight coplanar vortices, meeting at an angle of $\pi/4$ with alternating polarities in a cylindrical octagonal computational box, form a fixed point with a local structure

$$\Psi_8(x,y,z) \approx yx^3 - xy^3 + i(\zeta^3 z). \tag{6}$$

The relaxed, fully nonlinear fixed point found by the DGPE process is shown in Fig. 5(a). Note that (5) and (6) are members of a likely family of 4, 6, 8, etc., coplanar half-vortices joining at the origin. This family can easily be computed in the linearized version.

Further, as shown in Fig. 5(b), we have found a 3D fixed point that satisfies the advection analysis in a body centered cubic geometry. The local linear structure of this fixed point is

$$\Psi_{8\mathrm{BCC}}(x,y,z) \approx x^2 + y^2 - 2z^2 + i(x^2 + z^2 - 2y^2). \tag{7}$$

In conclusion, we present an identification of a family of phase singularities and topology-changing events permitted in complex fields with vortex reconnection in the Gross-Pitaevskii equation. Quantum turbulence decay may be more deeply understood as a relaxation of the topology of the complex order parameter, permitted only through ring decay and vortex reconnection. A method for finding appropriate initial conditions is outlined, with an application to find fixed points of the Gross-Pitaevskii equation. A host of reconnection fixed points have been identified numerically, one of which directly counters previous claims of pyramidal vortex reconnection geometry.[1,14]

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